

# **Developments of HFB solvers and continuum effects in deformed drip-line nuclei**

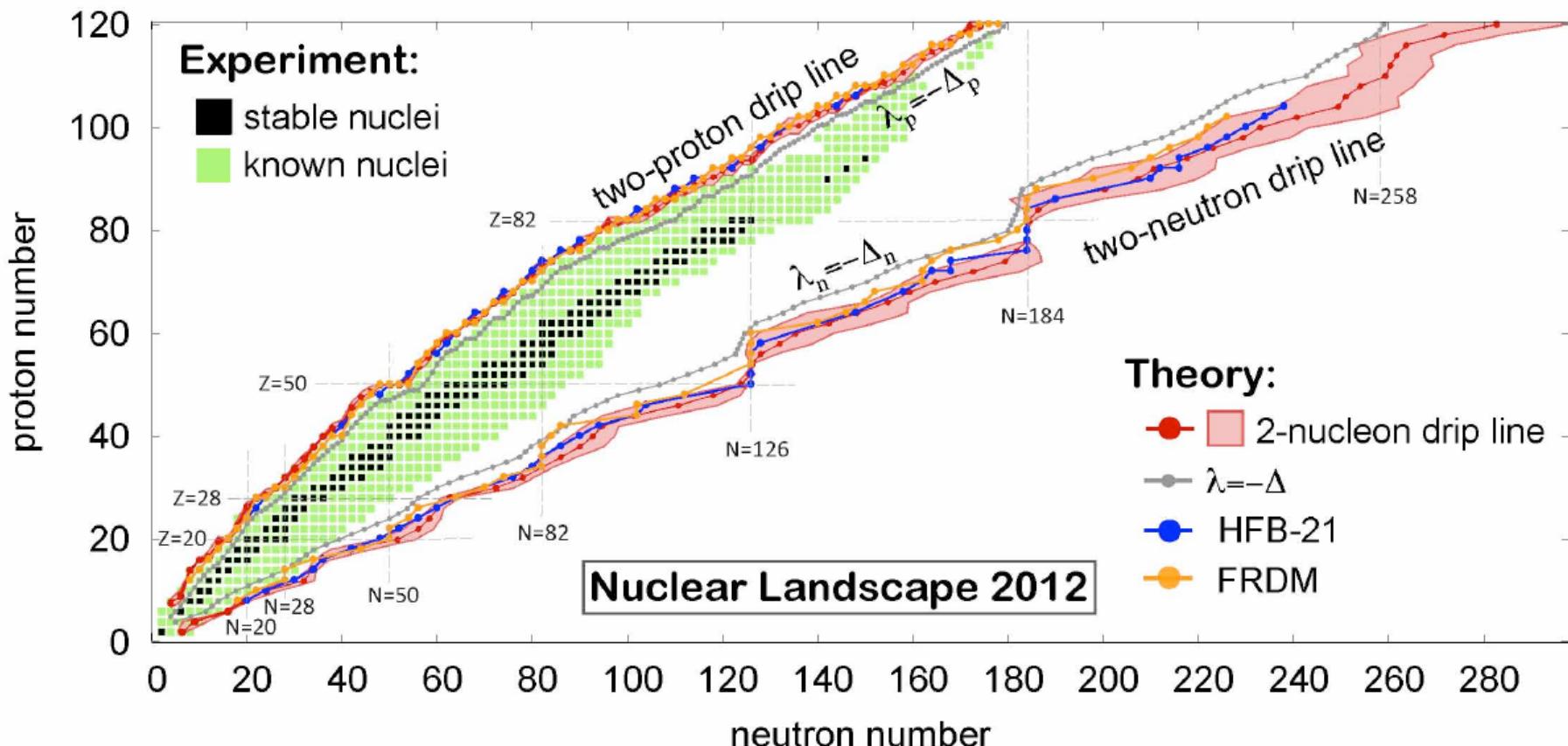
**NS12 conference, Argonne, Aug.16, 2012**



Junchen Pei (School of Physics, Peking University)

# Physics of drip-line nuclei

RNB facilities offer unprecedented opportunities to access unstable nuclei  
Challenging theoretical approaches

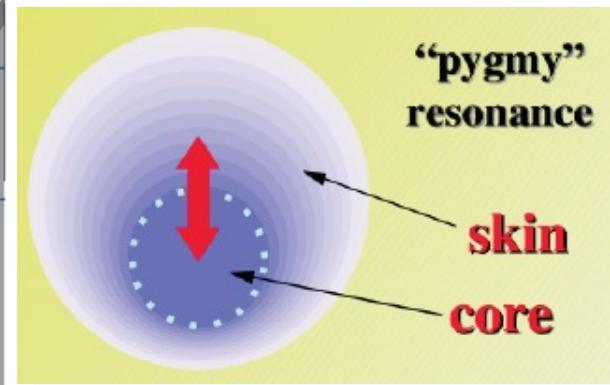
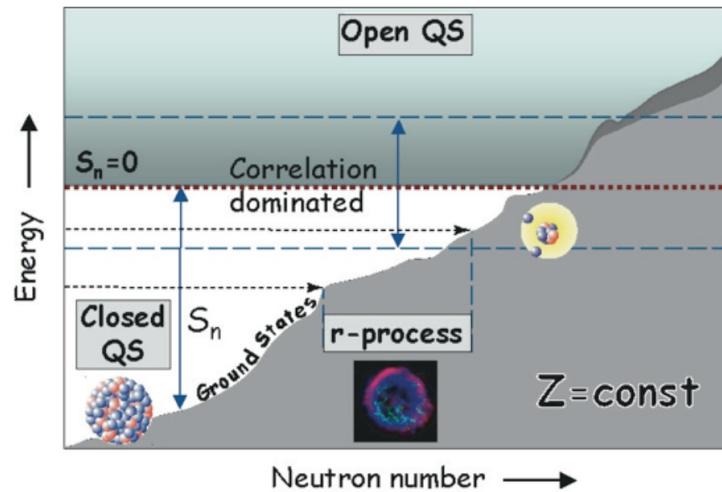
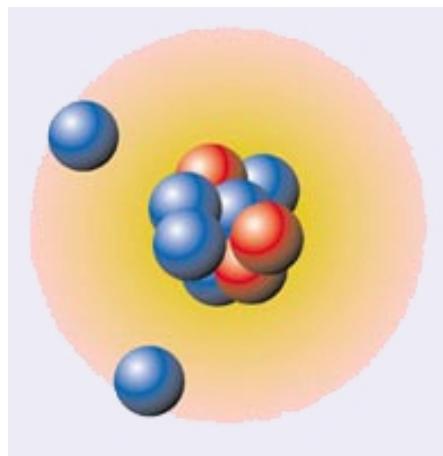


From J. Erler et al., Nature, 486, 509(2012)



# Physics of drip-line nuclei

- Weakly-bound systems: density diffuse, halo structures, deformed halo
- Continuum couplings become important
- Noval collective excitation modes
- Nuclear astrophysics: e.g., r-process
- Testing ground for new effective interactions: UNEDF, 3-body forces
- Islands beyond drip-lines, e.g., neutron stars



# HFB Theory

Hartree-Fock-Bogoliubov includes generalized quasi-particle correlations; while BCS is a *special* quasiparticle transformation only on conjugate states.

$$\beta_K^+ = \sum_i (u_{iK} c_i^+ + v_{iK} c_i^-) \quad \text{HFB G.S.: } \beta_K |\Psi\rangle = 0$$

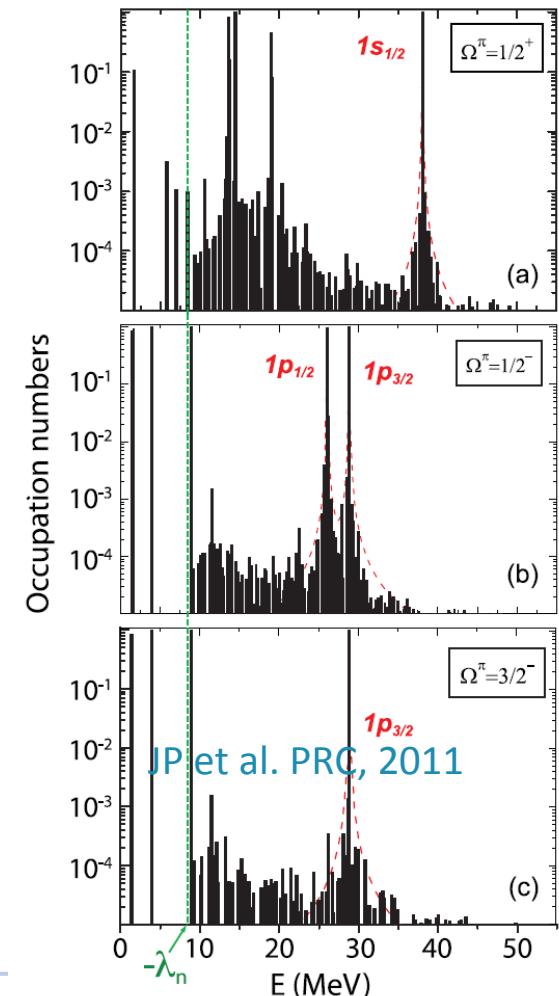
$$\alpha_k^+ = u_k c_k^+ - v_k c_k^- \quad \text{BCS G.S.: } \alpha_k |0\rangle = 0$$

- The general HFB equation(or BdG)

$$\begin{bmatrix} h_\uparrow(\mathbf{r}) - \lambda_\uparrow & \Delta(\mathbf{r}) \\ \Delta^*(\mathbf{r}) & -h_\downarrow(\mathbf{r}) + \lambda_\downarrow \end{bmatrix} \begin{bmatrix} u_i(\mathbf{r}) \\ v_i(\mathbf{r}) \end{bmatrix} = E_i \begin{bmatrix} u_i(\mathbf{r}) \\ v_i(\mathbf{r}) \end{bmatrix}$$

**HFB** is superior to **BCS** for describing weakly-bound systems where continuum coupling becomes essential

Also widely applications in describing Fermi gas, neutron stars



# HFB Solutions

- HFB resonances are embedded in the continuum

- Diagonalization on single-particle basis
- Direct diagonalization on coordinate-space lattice
- Outgoing boundary condition: difficult for deformed cases

- Coordinate-space HFB: weakly-bound systems and large deformations

- The HO basis has a Gaussian form  $\exp(-ar^2)$  that decays too fast, while the density distribution decays exponentially  $\exp(-kr)$ .
- Bound states, continuum and embedded resonances are treated on an equal footing;  $L^2$  discretization leads to a very large configuration space(*box-size dependent!*)
- Very accurate for describing weakly-bound nuclei with diffused density distributions; nuclear fission processes
- Providing precise inputs for QRPA, for describing excited states



# Deformed Coordinate-space HFB

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- Development issues: expensive, therefore parallel is essential; and most heavy dripline nuclei are deformed
- 2D HFB based on B-splines, finite-difference method
  - *V. E. Oberacker, A. S. Umar, E. Terán, and A. Blazkiewicz, PRC 68, 064302*
  - *J. C. Pei, M. V. Stoitsov, G. I. Fann, W. Nazarewicz, N. Schunck, and F. R. Xu, PRC 78, 064306 (Much faster and be able to calculate heavy nuclei)*
  - *H. Oba, M. Masto, Prog.Theor.Phys.120:143-157,2008*
- 3D MADNESS-HFB with Multi-wavelets techniques and sophisticated parallel techniques
  - *J.C. Pei, G.I. Fann, R.J. Harrison, W. Nazarewicz, J. Hill, D. Galindo, J. Jia, arXiv:1204.5254*
- Computing capability's exponential development: multi-core+GPU



# High energy continuum states

- High-energy approximation (local density approximation)  
 $u(\mathbf{r}) \rightarrow u(\mathbf{p}, \mathbf{r})e^{i\hbar\phi(\mathbf{r})}$ ,  $v(\mathbf{r}) \rightarrow v(\mathbf{p}, \mathbf{r})e^{i\hbar\phi(\mathbf{r})}$
- This approximation works for HFB-popov equation for Bose gas; works for Bogoliubov de Gennes equations for Fermi gas.

*J. Reidl, A. Csordas, R. Graham, and P.Szepfalusy, Phys. Rev. A 59, 3816 (1999)*

*X.J. Liu, H. Hu, P.D. Drummond, Phys. Rev. A 76,043605 (2007)*

- We follow this approximation for Skyrme HFB, to separate continuum contributions in 3D coordinate-HFB calculations(**motivation**).

$$\left( \frac{\hbar^2 p^2}{2M^*} + V(\mathbf{r}) - \lambda \right) u(\mathbf{p}, \mathbf{r}) + \Delta(\mathbf{r}) v(\mathbf{p}, \mathbf{r}) = \epsilon(\mathbf{p}, \mathbf{r}) u(\mathbf{p}, \mathbf{r})$$

$$\left( \frac{\hbar^2 p^2}{2M^*} + V(\mathbf{r}) - \lambda \right) v(\mathbf{p}, \mathbf{r}) - \Delta(\mathbf{r}) u(\mathbf{p}, \mathbf{r}) = -\epsilon(\mathbf{p}, \mathbf{r}) v(\mathbf{p}, \mathbf{r})$$

$$\epsilon(\mathbf{p}, \mathbf{r}) = \sqrt{\varepsilon_{\text{HF}}^2(\mathbf{p}, \mathbf{r}) + \Delta(\mathbf{r})^2} \quad \text{quasiparticle spectrum}$$

$$\varepsilon_{\text{HF}}(\mathbf{p}, \mathbf{r}) = \frac{\hbar^2 p^2}{2M^*(\mathbf{r})} + V(\mathbf{r}) - \lambda \quad \text{HF energy}$$

Derivatives of effective mass, spin-orbit terms omitted for high energy states



# Quasiparticle continuum contributions

- Continuum contributions to densities (from 30 to 60 MeV)

Box solutions ( $L^2$  discretization)

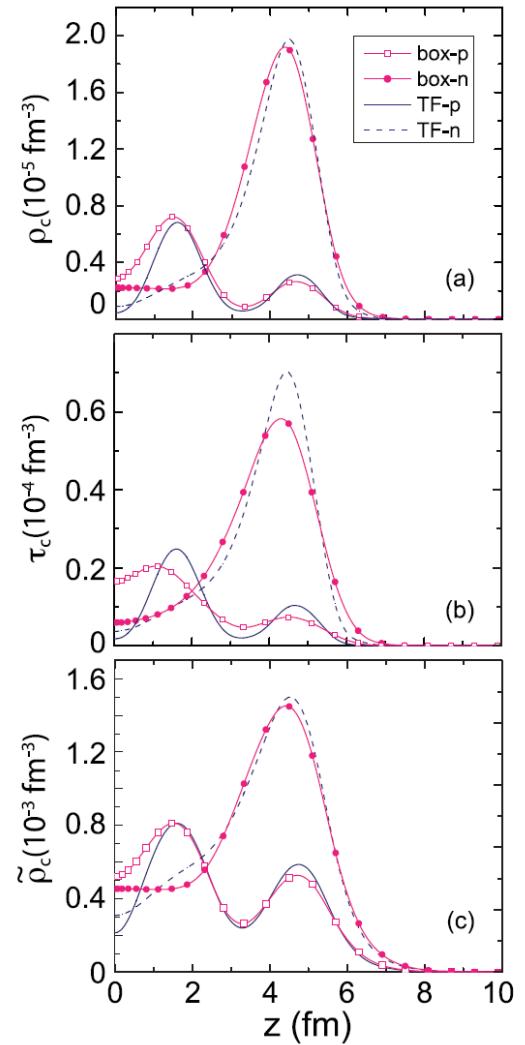
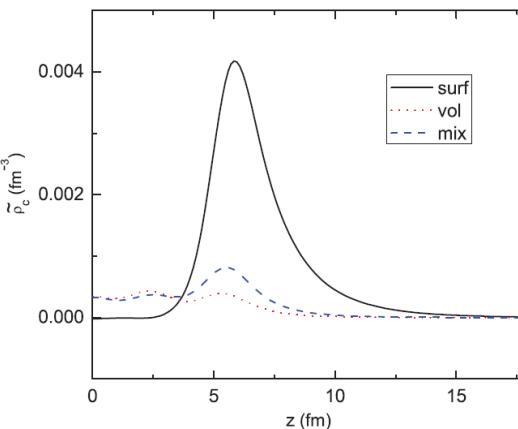
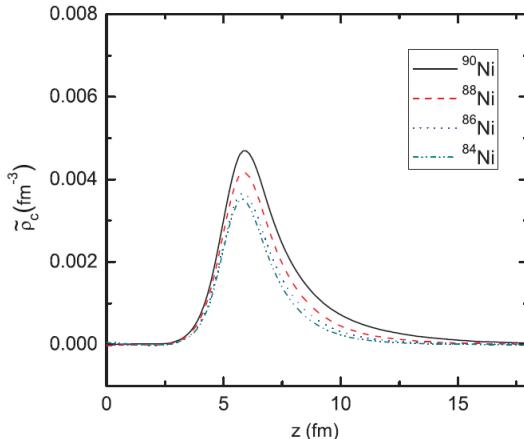
Local-density approximation (TF)

- What we see from the figures:

Local-density approximation works well for high energy continuum contributions.

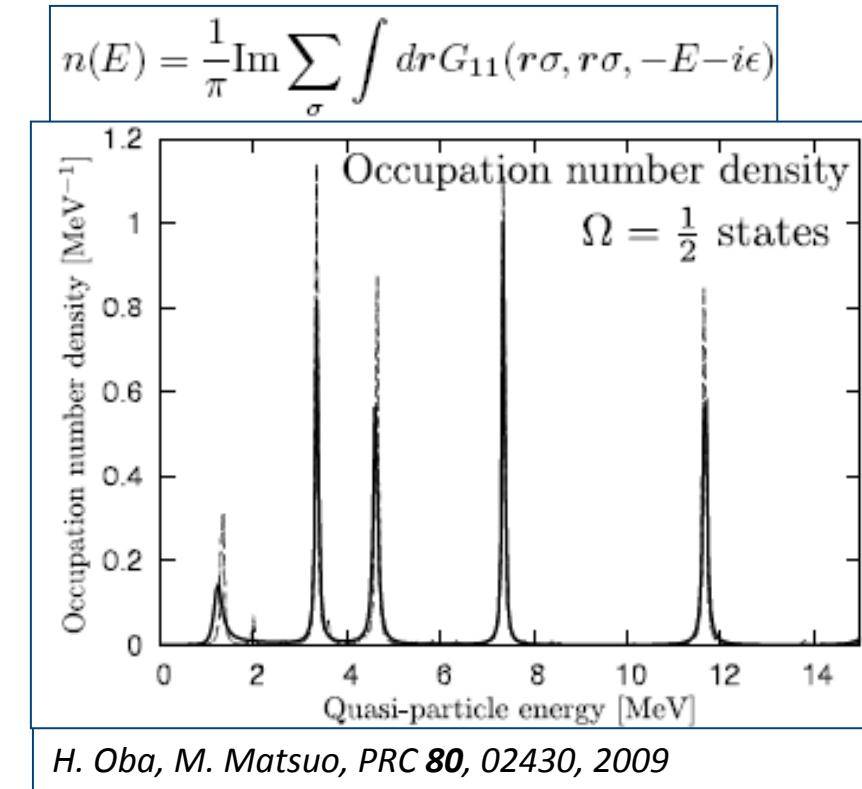
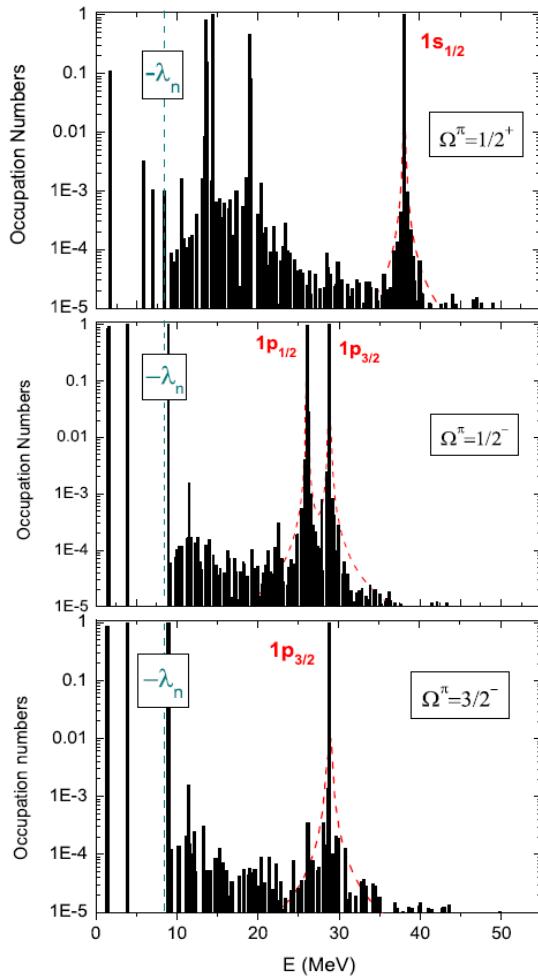
Continuum mainly impacts the  $pp$  channel.

Continuum contribution increases towards drip line



# HFB resonances

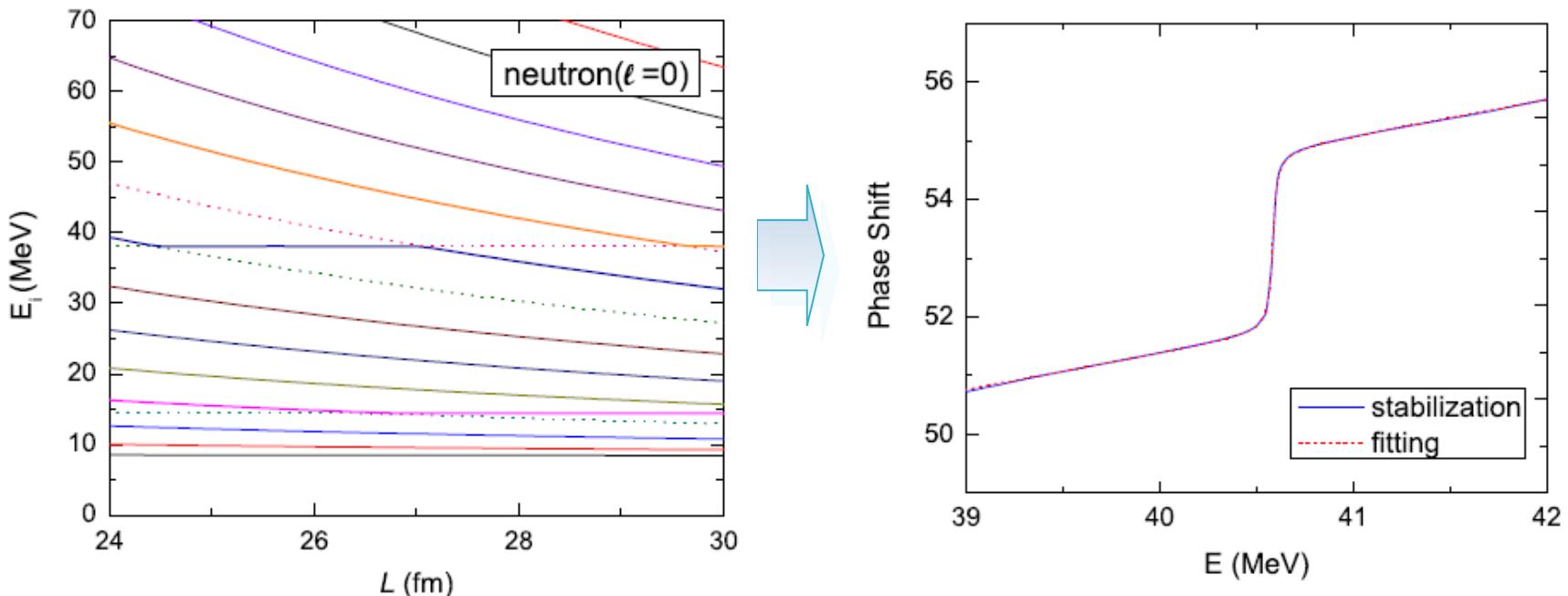
- Occupation probability and continuum level density



Occupation probability is related to the continuum level density, which corresponds to the Breit-Wigner shape



# HFB resonances in stabilization method



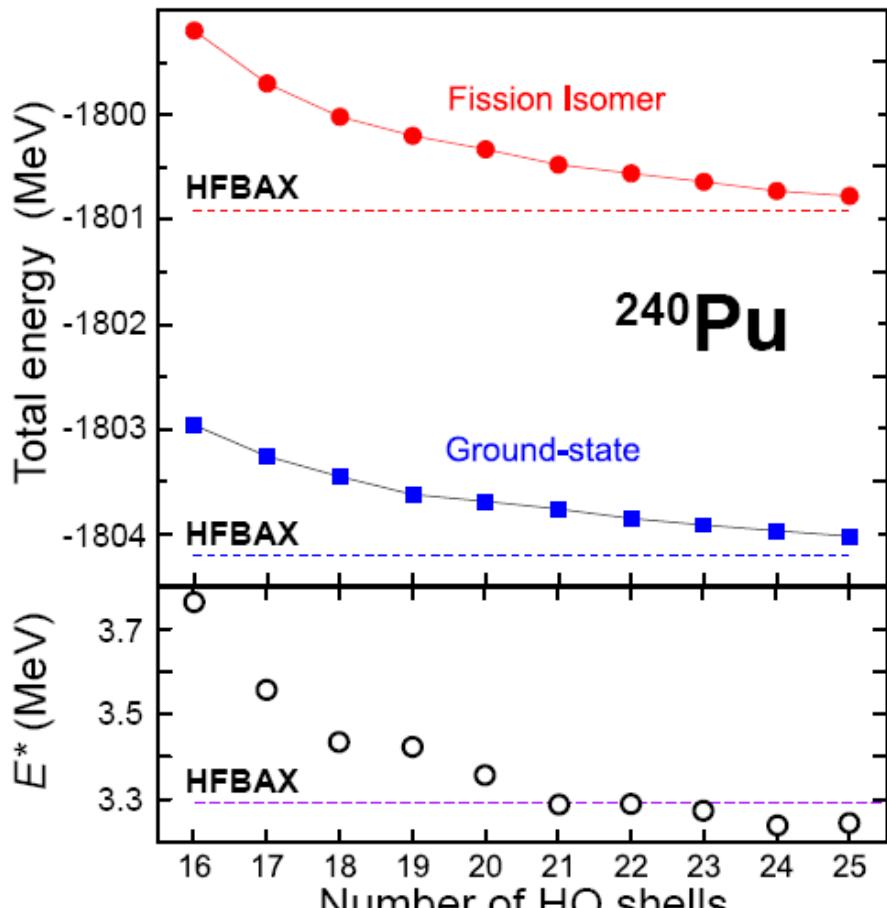
**Continuum level density:**  $\Delta(E) = \text{Tr}[\delta(E - H) - \delta(E - H_0)]$

**Phase shift:**  $\eta(E) = \pi \int_0^E \Delta(E') dE'$

- Box solutions are very precise compared to Gamow HFB approach
- Remarkable widths of HFB resonances in weakly-bound nuclei
- Provided an alternative way to study quasiparticle resonances



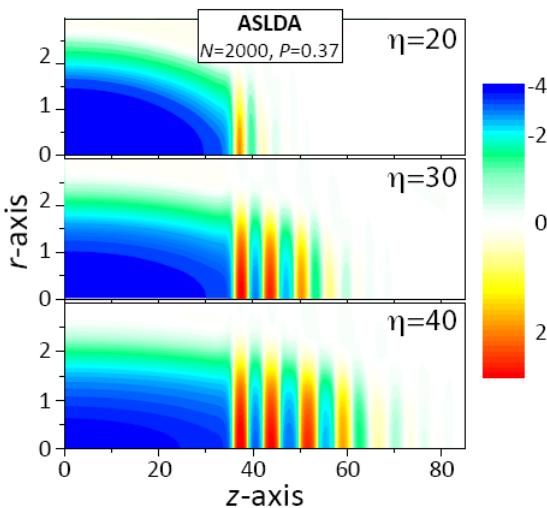
# Coordinate-space HFB benchmark



PRC 83, 034305 (2011)

Coordinate-space HFB is ideal for fission studies

Coordinate-space HFB has been applied to study highly elongated cold Fermi gases

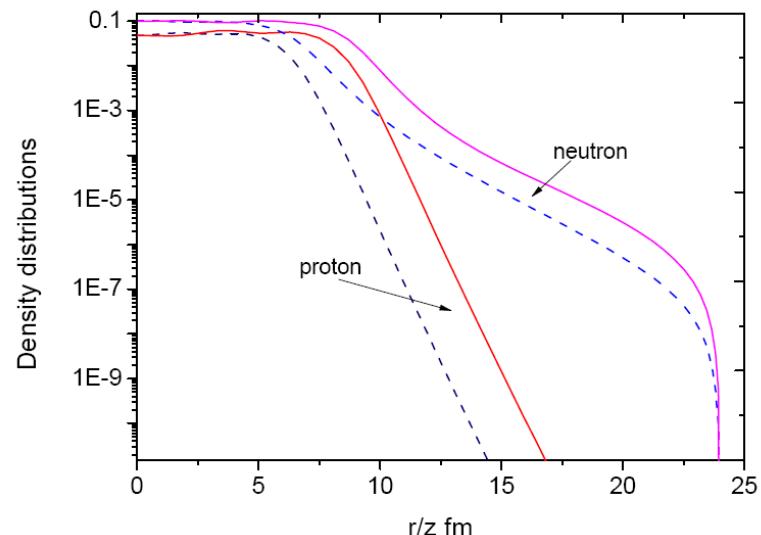
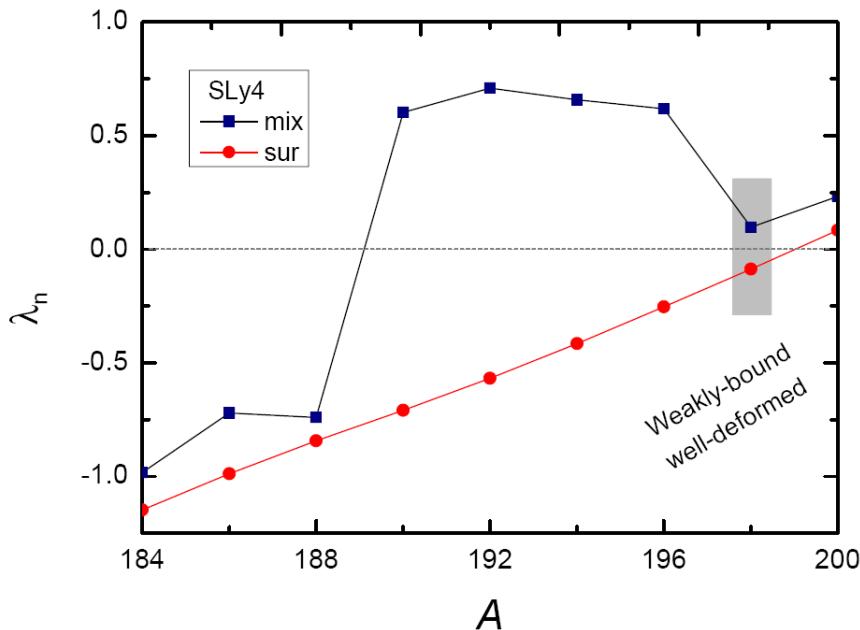


Phys. Rev A (R)(2010)



# Weakly-bound deformed nuclei

- Example: Nd isotopes near drip-lines are well deformed



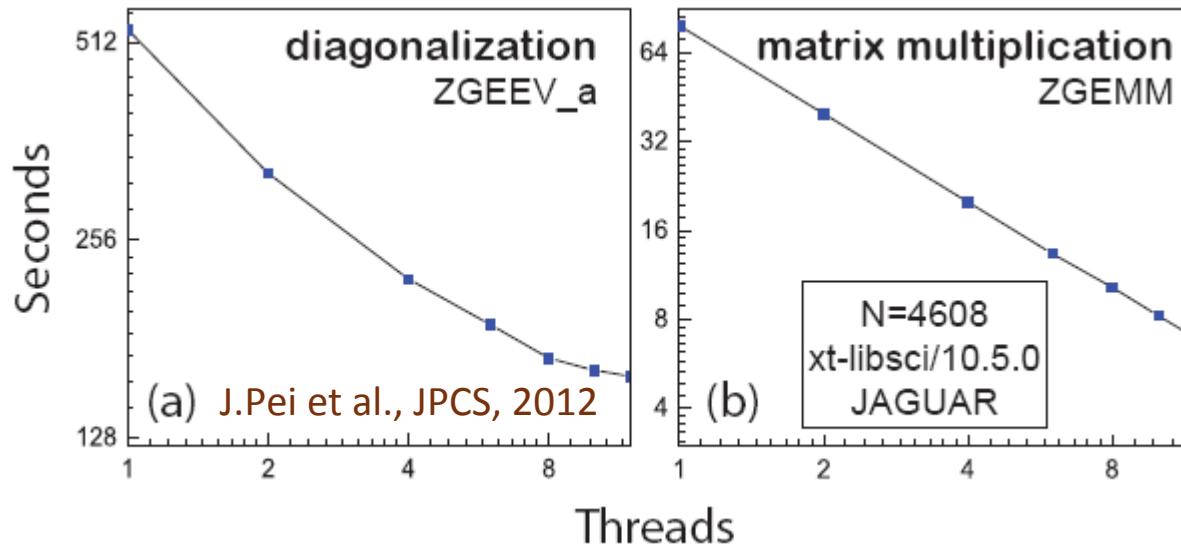
- For Nd198,  $\beta_2 \approx 0.25-0.35$ ,  
It gains more bounding in coordinates-space HFB , different from stable nuclei;  
Halo distribution is also well deformed, different from light nuclear halo Mg44
- Pairing treatment is another open issue

# Hybrid parallel calculation for large boxes

- MPI+OpenMP (400 cores for one nucleus takes 1 hour)

Computing different blocks on different nodes (MPI)

Multi-thread computing within a node(OpenMP)



- Very large box calculations for large systems, important for weakly-bound systems and cold atomic gases.

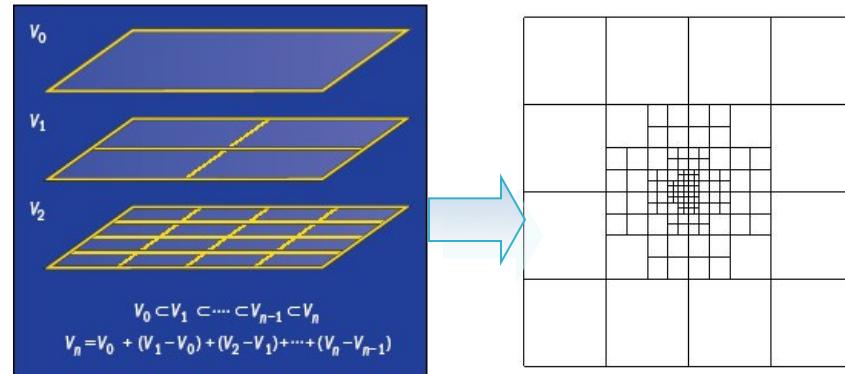
# 3D MADNESS-HFB

## Multi-resolution ADaptive Numerical Scientific Simulation

- **Multi-resolution:**

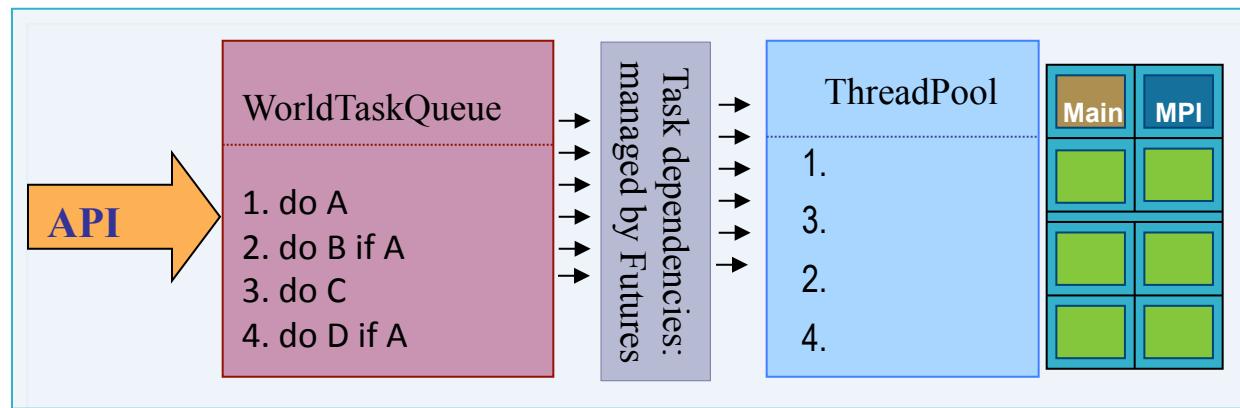
$$V_0 \subset V_1 \subset \dots \subset V_n$$

$$V_n = V_0 + (V_1 - V_0) + \dots + (V_n - V_{n-1})$$



- **CS infrastructure:**

Task-oriented: MPI, Global arrays, multi-threaded, futures (asynchronous computation), loadbalance



# Multi-Wavelets

## □ Decomposition

$$V_n^k = V_0^k + (V_1^k - V_0^k) + \cdots + (V_n^k - V_{n-1}^k)$$

$$V_{n+1}^k = V_n^k \oplus W_n^k \quad \text{Wavelet space at level } n$$

$$f^n(x) = \sum_{l=0}^{2^n-1} \sum_{i=0}^{k=1} s_{il}^n \phi_{il}^n(x) \quad \text{Scaling function expansion: expensive}$$

$$V_n^k = V_0^k \oplus W_0^k \oplus W_1^k \oplus \cdots \oplus W_{n-1}^k$$

$$f^n(x) = \sum_{i=0}^{k-1} s_{i0}^0 \phi_{i0}^0(x) + \sum_{n=0, \dots} \sum_{l=0}^{2^n-1} \sum_{i=0}^{k-1} d_{il}^n \psi_{il}^n(x)$$

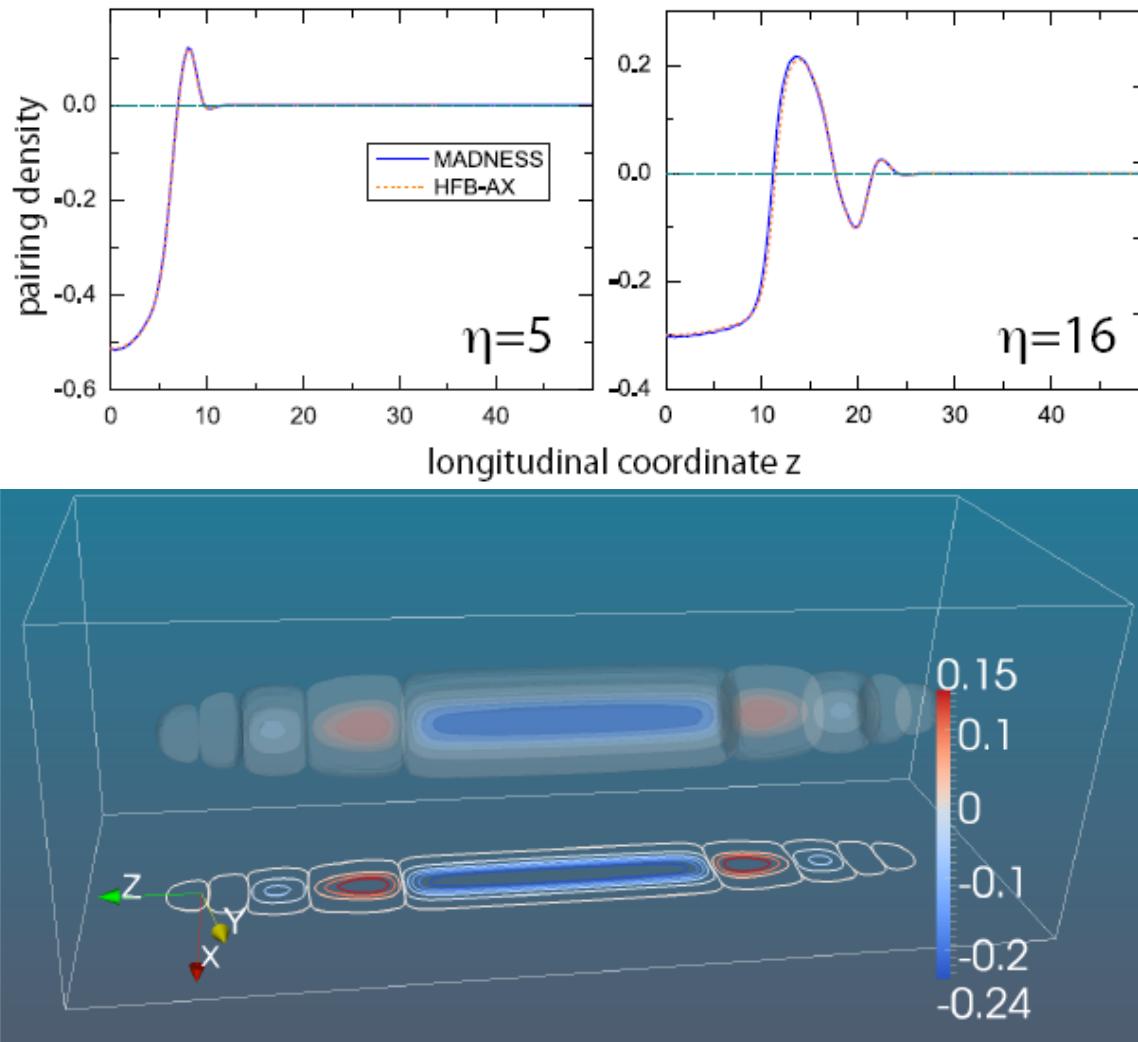
## □ Transformation

$$\begin{pmatrix} \phi_l^n(x) \\ \psi_l^n(x) \end{pmatrix} = \begin{pmatrix} H^{(0)} & H^{(1)} \\ G^{(0)} & G^{(1)} \end{pmatrix} \begin{pmatrix} \phi_{2l}^{n+1}(x) \\ \phi_{2l+1}^{n+1}(x) \end{pmatrix} \quad \|d_l^n\|_2 \leq \epsilon 2^{-nd/2}$$

## □ Truncation



# 3D MADNESS-HFB calculations of Fermi gases



J.P. et al, JPCS, (in press), 2012



# Summary and to do list

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- Deformed coordinate-space HFB is accurate not only for density diffuse structures but also for resonant continuum effects; Thomas-Fermi approximation is verified.
- Coordinate-space HFB is ideally suitable for describing weakly bound nuclei in large boxes by using hybrid parallel computing.
- 3D MADNESS HFB calculations can be done for light nuclei at the moment and TF approximation is very useful to reduce computation expenses

## To be done:

- Fast convergence has to be implemented for 3D MADNESS HFB calculations of heavy nuclei
- It will be interesting to looking for continuum effects in excited states, such as Pygmy resonances based on QRPA

Collaborators: W. Nazarewicz, A. Kruppa, G. Fann, F.R. Xu





Thanks for your attention!